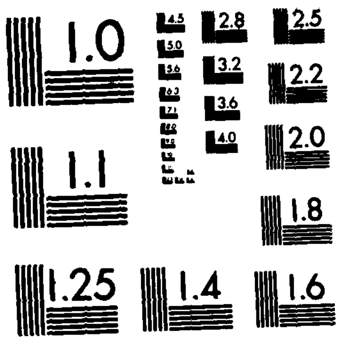
AD-A126 460 INTERFACIAL CHEMICAL REACTIONS AND TRANSPORT PHENOMENA IN FLOW SYSTEMS(U) YALE UNIV NEW HAVEN CT HIGH TEMPERATURE CHEMICAL REACTION ENG.. D E ROSNER JAN 82 1/1

UNCLASSIFIED AFOSR-TR-83-0127 F49620-76-C-0020 F/G 20/4 NL

END
FILMED
DTIC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: AFOSR-TR- 83-0127	2. GOVT ACCESSION NO.
3. RECIPIENT'S CATALOG NUMBER	
4. TITLE (and Subtitle): INTERFACIAL CHEMICAL REACTIONS AND TRANSPORT PHENOMENA IN FLOW SYSTEMS	5. TYPE OF REPORT & PERIOD COVERED: FINAL 1 Jul 76 - 30 Nov. 81
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): DANIEL E. ROSNER	8. CONTRACT OR GRANT NUMBER(s): F49620-76-C-0020
9. PERFORMING ORGANIZATION NAME AND ADDRESS: YALE UNIVERSITY, DEPT OF CHEMCIAL ENGINEERING, NEW HAVEN, CT 06520	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: 61102F 2308/A2
11. CONTROLLING OFFICE NAME AND ADDRESS: AIR FORCE OFFICE OF SCIENTIFIC RESEARCH/NA, BOLLING AFB, DC 20332	12. REPORT DATE: January 1982
	13. NUMBER OF PAGES: 8
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report): UNCLASSIFIED
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for Public Release; Distribution Unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

DTIC ELECTE APR 6 1983 S D

D

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

DEPOSITION	MASS TRANSFER	CONVESTIVE DIFFUSION
ENERGY TRANSFER	COMBUSTION	THERMAL DIFFUSION
FOULING	INERTIAL IMPACTION	THERMOPHORESIS
HETEROGENEOUS CATALYSIS	FLOW REACTORS	TURBINE BLADES

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report summarizes the results of a basic research program in the High Temperature Chemical Reaction Engineering (HTCRE) Laboratory at Yale University. Dealing broadly with chemical and physical phenomena at/near interfaces in high temperature systems, during this reporting period we have obtained further results in the areas of thermal diffusion effects on vapor and small particle mass transport across nonisothermal boundary layers, and inertial effects on particle deposition.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

AFOSR-TR AFOSR-TR- 83-0127

January 1982

Final ~~INTERIM~~ REPORT

to

U. S. AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
Bldg. 410, Bolling Air Force Base
Washington, D. C. 20332

Contract No. F49620-76-C-0020

INTERFACIAL CHEMICAL REACTIONS AND TRANSPORT PHENOMENA IN FLOW SYSTEMS

Principal Investigator: Daniel E. Rosner

Period Covered: 1 October 1980 - 30 November 1981

High Temperature Chemical Reaction Engineering Laboratory
Yale University
Department of Chemical Engineering
P. O. Box 2159YS
New Haven, Connecticut 06520, USA

APPROVED FOR PUBLIC RELEASE: DISTRIBUTION UNLIMITED

CONTENTS

TABLES

1. Introduction:

This interim report summarizes a 14-month basic research program in the High Temperature Chemical Reaction Engineering (HTCRE) Laboratory at Yale University. Our concern is primarily with chemical and physical phenomena near interfaces in high temperature systems, and during this reporting period we have obtained further results in the areas of i) surface-catalyzed combustion, ii) the influence of particle thermophoresis on mass transport across nonisothermal boundary layers, and iii) inertial effects on particle deposition to cooled targets in convective flow. These phenomena constitute a central part of advanced engineering systems containing dispersed condensed phases, or where the condensed phases are used for fluid confinement. The design of advanced propulsion systems requires fundamental data in these broad categories, and it is hoped that the research results and techniques reviewed here will continue to be widely used in the fields of aeronautical, metallurgical, chemical, and mechanical engineering (see Section 5 and 6).

Because of the current or impending availability of our papers in the archival scientific and/or engineering literature, detailed summaries of their contents would be redundant. However, the nature of the information resulting from this program is conveyed in Section 7 *via* a listing of publications prepared and/or appearing since 1 October 1980. If required, reprints of these papers can be obtained by writing the author. Information on further applications of this work by other workers (regardless of their field) will be especially welcome. Also included is a listing of the 16 talks given during this reporting period, verbally communicating our techniques and results.

The author would also like to acknowledge the many valuable contributions to this program made by his colleagues in the Chemical Engineering Department of Yale University, and elsewhere. This includes Professors Nordine and Halpern, my graduate students: J. Fernandez de la Mora, R. Israel, S. Gokoglu, R. Nagarajan, my postdoctoral research colleagues: R. Atkins and S. S. Kim, and the other research associates listed in Section 8.

2. Technical Objective:

Materials technologies for turbine blades and combustion chambers, re-entry heat shields and rocket nozzles are seriously lacking in both theoretical understanding and reliable experimental data on basic gas-solid reactions at high temperatures and laws governing mass/heat exchange with the surface. This research will provide to systems and materials engineers theoretical understanding and fundamental data on interfacial rate processes, both for gas-surface and gas-particle interactions, with emphasis on high temperautre (high performance) systems.

3. Approach:

We are currently developing theoretical methods to generalize the laws of convective mass and energy transfer to include thermophoresis (particle drift down a temperature gradient), and particle inertial effects in systems with heterogeneous chemical reaction, phase change or particle (e.g. soot, ash) deposition on actively cooled solids (e.g. gas turbine vanes, blades). Experimental work will develop new optical methods for studying small particle (soot, ash) deposition to colled targets in combustion gases and extend the capability of the filament flow reactors to the catalytic oxidation of vapor fuels.

Table 1

Subject Matter of Papers Listed in Section 7

Subject[a]	Papers[a]	Talks[a]
gas turbine blade fouling and corrosion	3,7,12	1,2,3,4,7,11
aerosol capture by inertial impaction	1,3,4,5,8,12	1,2,3,7,14
experimental techniques: deposition from combustion gases	2,10,11,14	1,5,6,7,12
surface-catalyzed combustion	9	15
mass transport across transpiration-cooled boundary layers	3,5	15
thermal diffusion and viscous dissipation effects on convective mass transport	1,3,5,7,13	15
chemical energy accommodation at catalytic surfaces	6	9,10

[a]Titles and complete bibliographic information are given in Section 7.

4. Progress (Selected Results, Conclusions) October 1980-December 1981

Ongoing research on thermophoretically and inertially modified vapor and small particle deposition reveals that:

R1. Our preliminary H_2/air surface-catalyzed combustion experiments demonstrate that thermal (Soret) diffusion enhances the transport rate of the light fuel H_2 to the hot catalyst surface by more than a factor of 1.15.

R2. Soot, salt or ash particle deposition by convective diffusion on actively cooled surfaces (e.g. GT blades) can be increased by about 100-fold due to thermophoresis (*i.e.*, particle drift down a temperature gradient.

R3. Systematic comparisons with the results of exact solution to the boundary layer equations reveal that our new "pseudo-blowing/source" correlation successfully predicts the effects of thermal (Soret) diffusion transpiration and/or viscous dissipation on mass transfer rates in laminar or turbulent forced convection situations of interest in the fields of soot or ash deposition in combustors, or gas turbine stages, surface-catalyzed combustion, chemical vapor deposition (CVD) systems, is now being generalized to allow the treatment of simultaneous particle phoretic effects (e.g. sedimentation, centrifugal drift, electrostatic precipitation, etc.).

R4. Particle capture date at supercritical Stokes' numbers can be correlated in terms of an effective Stokes number which incorporates the effects of non-Stokes' particle drag, collector geometry, and gas compressibility.

R5. For inertial particle deposition, local particle enrichment or depletion, phenomena can occur even at subcritical Stokes' numbers. An Eulerian particle deposition approach can be used to predict deposition rate distributions on curved targets and extended, using a Fokker-Planck formulation, to explain aerodynamic isotope separation phenomena in low density gases.

R6. Optical methods (e.g. change in surface reflectivity) appear to be promising for rapid measurements of deposition (salt, "ash") from seeded combustion gases. Preliminary measurements of micron-sized TiO_2 and MgO-particle deposition reveal significant effects of thermophoresis for radiation cooled ribbon targets in flat hydrocarbon/air flames.

5. Technological Significance, Relevance:

A reliable basis for predicting vapor and particle deposition rates from combustion gases should now enable more rational gas turbine fuel purity standards to be set, and allow deposition/corrosion control systems to be selected and optimized. Results of this phase of our research will allow future aircraft gas turbines to be designed to operate efficiently, reliably and economically, using a broader range of liquid fuels, and over a wider variety of environmental conditions (including the ingestion of marine air or desert dust).

6. Scientific Applications, Research Implications:

Results of this program continue to be of use to research in the following areas:

* Correlation of heat exchanger tube fouling behavior in pulverized coal-fired combustors (EXXON).

* Hot corrosion and aircraft icing studies (NASA-Lewis Research Labs).

* Development of on-line salt dew-point and deposition rate detectors (Argonne National Laboratories).

* Deconvolution of observed particle size spectra to infer mainstream ("undisturbed") size distributions (e.g. soot in flames) (all combustion research labs).

* Feasibility studies of a new class of low pressure drop particle filters for gas turbines (U. S. Naval Ship Engineering Center, Philadelphia).

* Exploitation of thermophoresis in the production of optically graded light communication pipes (Bell Labs).

* Use of mathematical methods to predict surface-catalyzed combustion rates in forced convection boundary layer situations (Grench researchers Garo, Ledoux, Gousebet et al.).

* Performance of Space Shuttle Orbiter thermal protection system materials (NASA-Houston).

* Gasification kinetics of pyrolytic graphite AGT combustor liners by atomic oxygen (H. Nelson, J. Holsom, A. Bruns, McDonnel-Douglass, St. Louis, MO).

* Interpretation of small particle inertial impactor performance under low pressure, transonic jet conditions (Herring, Flagan et al.).

7. Bibliography (October 1980 - December 1981:

7.1 Papers in Print

P1. Fernandez de la Mora, J. and Rosner, D.E.: "Inertial Deposition of Particles Revisted and Extended; Eulerian Approach to a Traditionally Lagrangian Problem". J. Physiochemical Hydrohynamics (Pergamon 2, 1-21 (1981).

P2. Rosner, D.E. and Seshadri K.: "Experimental and Theoretical Studies of the Laws Governing Condensate Deposition from Combustion Gases." Fifteenth International Symposium Combustion, (The Combustion Inst., Pittsburgh, Pa.), pp. 1385-1394 (1981).

P3. Rosner, D.E. and Fernandez de la Mora, J.: "Discussion of Deposition in PFBC Power Plant Turbines." Trans. ASME, J. Engineering for Power, 103, 558-560 (July (1981)).

P4. Fernandez de la Mora J., Mercer, J., Rosner, D.E. and Fenn, J.B.: "Simplified Kinetic Treatment of Heavy Molecule Velocity Persistence Effects: Application to Species Separation" in Rarefied Gas Dynamics (S.S. Fisher, ed.) Vol. 74 Bigness in Astronautics and Aeronautics, AIAA (NYC) 1981, pp. 617-626.

P5. Fernandez de la Mora, J.: Deterministic and Diffusive Mass Transfer Mechanisms in the Capture of Vapor and Particles, PhD Dissertation, Yale University, (December (1980)).

7.2 Papers Submitted, or in Press

P6. Halpern, B. and Rosner, D.E.: "Incomplete Energy Accommodation in Surface Catalyzed Reactions" in Heterogeneous Atmospheric Chemistry (monograph, in press 1982).

P7. Rosner, D.E. and Fernandez de la Mora, J.: "Particle Transport Across Turbulent Nonisothermal Boundary Layers." ASME Transactions - J. Engineering for Power (in press, summer, 1982).

P8. Israel, R. and Rosner, D.E.: "Use of a Generalized Stokes Number to Determine the Aerodynamic Capture Efficiency of Non-Stokesian Particles from a Compressible Gas Flow." Yale HTCRE Lab Reprint (June 1981); Aerosol Science and Technology (submitted 1982).

P9. Rosner, D.E.: Energy, Mass and Momentum Transport in Chemically Reacting Fluids. J. Wiley — Exxon Research and Engineering Textbook Series, (in press 1982).

P10. Seshadri, K. and Rosner, D.E.: "Polarization (Ellipsometric Measurement of Condensate Deposition and Evaporation Rates in Salt/Ash-Containing Gases." Combustion and Flame (in press 1981).

P11. Seshadri, K. and Rosner, D.E.: "Optical Methods of Dew Point and Deposition Rate Measurements in Salt/Ash-Containing Combustion Gases —1. $B_2O_3(\ell)$ Deposition Rates by the Interference Method and Comparison with Theory." Amer. Inst. Chem. Engineers J. (in press 1982).

P12. Fernandez de la Mora, J. and Rosner, D.C.: "Effects of Inertia on the Diffusional Deposition of Small Particles to Spheres and Cylinders at Low Reynolds Numbers." J. Fluid Mechanics (submitted 1981).

P13. Rosner, D.E., Israel, R., Sydney, A.: "Effect of Thermophoresis on the Minimum Attainable Aerosol Diffusional Deposition Rate Before the Onset of Inertial Impaction." Yale HTCRE Laboratory Preprint, (May 1981).

P14. Rosner, D.E. and Atkins, R.M.: "Experimental Studies of Salt/Ash Deposition Rates from Combustion Products Using Optical Techniques." Proc. Engineering Foundation Int. Conference on Research into Fouling and Slagging Due to Impurities in Combustion Gases. (R. Bryers, ed.) (in press 1982).

7.3 Papers Presented

T1. Rosner, D.E.: "Experimental and Theoretical Studies of the Laws Governing Condensate Deposition from Combustion Gases." Seminar, M.I.T. — Chemical Engineering Dept., October 23, 1981.

T2. "Prediction of Thermophoretic Diffusion Effects in Flow Systems, With Applications to Materials Processing." Invited paper presented at 18th Annual Meeting of the Society of Engineering Science, Brown Univ., Providence, RI, September 2-4 (1981); (Session on Heat and Mass Transfer in Materials Science).

T3. Anous, N.N. and Rosner, D.E.: "Condensate Deposition and Flow on Surfaces Exposed to Combustion Gases". Presented at the Final Conference - Summer Research Program, Engineering and Applied Science Yale University, New Haven, CT August 19, 1981.

T4. Vesenka, J. and Rosner, D.E.: "Influence of Transport Phenomena on Dew Points in Combustion Systems." Presented at the Final Conference - Summer Research Program, Engineering and Applied Science, Yale University, New Haven, CT, August 19, 1981, (with J. Vesenka, speaker).

T5. Eisenstein, S. and Rosner, D.E.: "Experiments on Alkali Sulfate Vapor Deposition from Combustion Gases." Presented at the Final Conference - Summer Research Program, Engineering and Applied Science, Yale University, New Haven, CT, August 19, 1981, (with S. Eisenstein speaker).

T6. Rosner, D.E. and Atkins, R.: "Experimental Studies of Salt/Ash Deposition Rates from Combustion Products Using Optical Techniques." Invited paper presented at the Engineering Foundation International Conference on Experimental Research into Fouling and Slagging Due to Impurities in Combustion Gases; Henniker, New Hampshire July 12-17, 1981.

T7. Rosner, D.E.: "Experimental and Theoretical Studies of the Laws Governing Condensate Deposition from Combustion Gases." CHE/ME Seminar, City College of New York May 18, 1981.

T8. "Current Research at Yale University ChE Department on Mass Transfer and Heterogeneous Kinetics in High Temperature Systems," General Electric Co. - Lighting Research and Technical Services Operations, Nela Park, Cleveland, Ohio, May 13, 1981.

"Recent Developments in Deposition Theory and Experiments," Seminar Presented at: NASA Lewis Research Center, Materials and Structures Lab, Cleveland, Ohio, May 13, 1981.

T9. "Experimental and Theoretical Studies of the Laws Governing Condensate Deposition from Combustion Gases," United Technologies Research Laboratories Seminar, E. Hartford, CT, April 28, 1981.

"Chemical Energy Accommodation in Simple Surface-Catalyzed Reactions," Presented at American Chemical Society meeting - Div. Colloid/Surface Chem., March 29 - April 3, 1981, Atlanta, Ga. (with B. Halpern, speaker).

T10. Halpern, B.L. and Rosner, D.E.: "Chemical Energy Accommodation in Simple Surface-Catalyzed Reactions." Amer. Chem. Soc. Div. Colloid/Surface Chemistry, Atlanta, Ga. Meeting March 29-April 3, 1981.

T11. Rosner, D.E.: "Deposition Phenomenon in Gas Turbines." Invited Panel Discussion: Amer. Soc. Mech. Engineers 26th Internat. Gas Turbine Conference, Session 72, Houston, TX March 12, 1981.

T12. "Experimental and Theoretical Studies of the Laws Governing Condensate Deposition from Combustion Gases," Seminar: Shell Dev. Co. - Westhollow Research Center, March 10, 1981.

"Combustion System Processes Leading to Corrosive Deposits," presented at the NACE Int. Conference on High Temperature Corrosion, San Diego, CA, March 2 - 6, 1981 (with F. Kohl, speaker and C.A. Stearns).

7.3 Papers Presented - continued

"Inertial and Thermophoretic Effects on the Capture of Fuel Ash Particles by Gas Turbine Blades," Invited Panelist, Session 72, VII - Deposition Effects on Gas Turbines - Panel Discussion, ASME 26th International Gas Turbine Conference and Exhibit, Houston, Texas, March 12, 1981.

T13. "Thermophoretic Diffusion Effects on Mass Transport Rates to/from Interfaces," Center for Fluid Mechanics Seminar, Brown University, Feb. 26, 1981.

T14. "Effect of Thermophoresis on the Minimum Attainable Aerosol Diffusional Deposition Rate before the Onset of Inertial Impaction," ACS/IEC - 81 Winter Symposium on Aerosol Systems, January 26 - 28 (1981).

T15. Rosner, D.E.: "Interfacial Chemical Reactions and Transport Phenomena in Flow Systems." Presented at 1981 AFOSR Contractor's Meeting on Air Breathing Combustion and Explosion Research, November 16-20, 1981 Clearwater Beach, Florida.

T16. "Mass Transfer from Combustion Gases," Paper No. 59a, presented at the AIChE 73rd Annual Meeting, November 16 - 20, 1980, Chicago, Ill.

8. Personnel Contributing to this Research:

Name	Status at Yale U.	Contribution
Rosner, D.E.	P.I.[a], Prof. ChE	Direct program on interfacial reaction/transport
Fernandez de la Mora, J.	PDRA[d]	Theory of particle transport
Halpern, B.	Asst. Prof. ChE	Energy transport experiments
Israel, R.	GRA[b]	Surface catalyzed H_2-combustion
Anous, N.	GRA-MSE	Condensate film flow theory
Nagaragan, R.	GRA-SRP[c]	Multicomponent vapor transport theory
Eisenstein, S.	SRP[c]	
Gokoglu, S.	GRA	Thermophoretic transport in boundary laye
Kim, S.S.	PDRA[d]	Aerosol deposition from flames
Atkins, R.	PDRA	Aerosol deposition from flames
Vesenka, J.	SRP	Dew point phenomena

[a]Principal Investigator

[b]Graduate Research Assistant

[c]Summer Research Program - Yale Engineering and Applied Science

[d]Postdoctoral Research Assistant

4 - 8

DTI